

# Investigation of Multiscale Non-equilibrium Flow Dynamics Under External Force Field

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The multiple scale non-equilibrium gaseous flow behavior under external force field is investigated. Both theoretical analysis based on the kinetic model equation and numerical study are presented to demonstrate the dynamic effect of external force on the flow evolution, especially on the non-equilibrium heat flux. The current numerical experiment is based on the well-balanced unified gas-kinetic scheme (UGKS), which presents accurate solutions in the whole flow regime from the continuum Navier-Stokes solution to the transition and free molecular ones. The heat conduction in the non-equilibrium regime due to the external forcing term is quantitatively investigated. In the lid-driven cavity flow study, due to the external force field the density distribution inside cavity gets stratified and a multiscale non-equilibrium flow transport appears in a single gas dynamic system. With the increment of external forcing term, the flow topological structure changes dramatically, and the temperature gradient, shearing stress, and external force play different roles in determination of the heat flux in different layers corresponding to different flow regime. Besides the non-Fourier's heat effect in the transition regime, such as the heat flux from cold to hot region in the absence of external field, the additional external force enhances the heat flux significantly along the forcing direction, which could trigger the gravity-thermal instability through the heat flow from the high potential cold region to the low potential hot region. At the same time, the wave propagation phenomena for the temperature field in the transition regime have been observed, which may be helpful for the modeling of hyperbolic heat evolution equation. Through the numerical experiment, it is clear that the external force plays an important role in the dynamic process of non-equilibrium heat transfer.

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## I. INTRODUCTION

The gas dynamic system under external force field is essentially associated with multiple scale nature due to the possible large variation of gas density, and the corresponding local Knudsen number. From the kinetic theory, as an example we can use the Bhatnagar-Gross-Krook (BGK) [1] equation to illustrate the effect of the external force on the variation of distribution function. The evolution of particle distribution function  $f(x_i, t, u_i, \xi)$  in space and time is described by

$$\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} + \phi_i \frac{\partial f}{\partial u_i} = \frac{g - f}{\tau}. \quad (1)$$

Here  $\xi$  is the internal variable for the rotation and vibration and  $\phi_i$  is the external forcing term. The Eq. (1) can be rewritten in the following form,

$$f = g - \tau(f_t + u_i f_{x_i} + \phi_i f_{u_i}). \quad (2)$$

Even with an initial Maxwellian distribution function, the free transport of particles during the traveling time between two successive collisions evolves the system away from equilibrium state. Under external force field, the particle acceleration or deceleration during this time interval results in a distortion of the distribution function in the velocity space simultaneously. Consequently, the particle collision takes effect to drive the system back to equilibrium state.

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However, in rarefied regime, the particle free transport and collision are loosely coupled due to a large particle collision time. Much complicated nonlinear dynamics due to particle transport, collision, and external force acceleration, will appear and presents a peculiar non-equilibrium flow behavior. Usually the non-equilibrium effects are expected to emerge in the highly dissipative regions, such as the shock and boundary layers. However, with the existence of external force field non-equilibrium gas evolution may spread to the whole flow system in a large scale.

It is noted that there is only limited study on non-equilibrium flow under external force field. Theoretically, the existence of external force field, such as gravity, introduces a characteristic length scale  $H \sim k_B T / m \phi$  [2], where  $k_B$  is the Boltzmann constant and  $m$  is the particle mass. It denotes a vertical distance over which the force field produces a significant effect on the gas evolution. For a gravitational system under laboratory condition or a micro-electro-mechanical system (MEMS) with geometric characteristic length  $L$ , the relation  $H \gg L$  holds naturally, and thus it is reasonable to omit the influence of external force. However, in the case where  $H$  is comparable to  $L$ , the effect of external force will appear. For example, let us consider a large scale cavity full of gases under gravitational field, such as the atmospheric environment. The external force will result in an observable variance of density in the cavity, and so is the variation of the particle mean free path and the local Knudsen number. Similar cases appear in small scale, but with large acceleration, such as material interface with shock impingement. Therefore, it is interesting to study the multiple scale non-equilibrium gas effect due to external force.

Different gas dynamic equations are used to describe the flow in different modeling scale. In hydrodynamic scale modeling, in 1822 Fourier [3] proposed a well-known phenomenological heat conduction law. Based on the Fourier's law and Newton's stress and strain relationship, the Navier-Stokes-Fourier (NSF) equations were constructed to describe the fluid motion and heat transfer in macroscopic scale. In the Navier-Stokes modeling, the fluid element picture is used and the intensive particle collisions prevent particle penetration between elements. In such a modeling, the diffusion formulation for heat flux introduces infinite propagation speed for the temperature field, which prevents its accurate description for the non-equilibrium heat transfer in rarefied flow [4]. The NS equations have no a clear modeling scale theoretically, and the boundary for its validation is not clearly defined. On the contrary, the Boltzmann equation is well defined on the modeling scales of particle mean free path and collision time, where the particle free transport and the collision can be described efficiently in an operator splitting way. It also limits the application of the Boltzmann equation to other scales, except resolving other scales all the way to the mean free path and particle collision time.

Physically, the valid application of distinguishable gas dynamic equations, such as NS and the Boltzmann, depends on their clear scale separation. However, for a system under external force field, the flow physics may vary continuously from the kinetic Boltzmann modeling in the upper rarefied layer to the hydrodynamic one in the lower dense region. Theoretically, in order to study the cross-scale flow physics, a valid modeling here should have a smooth scale variation between the kinetic and hydrodynamic ones. A unified approach is preferable to simulate such a system to capture a continuum spectrum of flow dynamics from rarefied to continuum one. The unified gas-kinetic scheme (UGKS) provides such a choice [5, 6]. The corresponding well-balanced scheme under external force field has been developed recently [7]. Through a coupled treatment of particle transport, collision, and external forcing effect in the evaluation of flux transport across a cell interface and inner cell flow evolution, a continuous spectrum of gas dynamic equations can be recovered [8]. In this paper, the well-balanced UGKS is employed to investigate the multiscale gas evolution under external force field.

Even under simple geometric condition, the cavity flow displays complex fluid mechanical phenomena with multiple scales, including shearing layers, eddies, secondary flows, heat transfer, hydrodynamic instabilities, and laminar-turbulence transition, etc [9]. Great efforts have been devoted to the study of the flow physics in different flow regimes as well. In the continuum regime, the cavity problem is a typical benchmark case for the validation of numerical algorithms for the NS solutions [9–13]. In rarefied regime, the direct simulation Monte Carlo (DSMC) [14] and kinetic Boltzmann solvers [15, 16] provide the benchmark solutions. Naris et al. [17] discretized a linearized BGK equation to investigate the rarefaction effect on the flow pattern and physical quantities over the whole range of the Knudsen number. Mizzi et al. [18] compared the simulation results from the Navier-Stokes-Fourier equations (NSF) with slip boundary conditions and the DSMC results in a lid-driven micro cavity case. John et al. [19] applied the DSMC, discovered counter-gradient heat transport in the transition regime, and investigated the dynamic effect from the expansion cooling and viscous dissipation on the heat transport mechanism. In all previous work, there is few study about the cavity flow under external force field. Due to the external force effect, the cavity flow becomes even more complicated with its non-equilibrium multiple scale nature. A few new phenomena, including the connection between the heat transfer and external force, and wave propagation of the temperature field, have been observed through this study.

This paper is organized as follows. The basic kinetic theory and the analysis of the influence of external force on the macroscopic flow transport are presented in Section 2. The well-balanced unified gas-kinetic algorithm under external force field is introduced in Section 3. Section 4 presents the numerical experiments and discussion on the non-equilibrium flow transport and heat transfer in different flow regimes. The last section is the conclusion.

## II. KINETIC ANALYSIS ON THE EXTERNAL FORCE

The macroscopic flow transport and heat transfer have a close relationship with the particle motion in the kinetic scale. In this section, we use the BGK equation to illustrate the influence of external force on a near-equilibrium gas dynamic system. For simplicity, the one-dimensional case is considered first.

Notice that Eq. (1) can be rewritten in a successive form:

$$f = g - \tau \frac{Df}{Dt} = g - \tau \frac{D}{Dt} \left( g - \tau \frac{Df}{Dt} \right) = \dots, \quad (3)$$

where  $D/Dt$  is the material derivatives. The  $\tau = \mu/p$  is the collision time, and the Maxwellian distribution  $g$  writes,

$$g = \rho \left( \frac{\lambda}{\pi} \right)^{\frac{K+1}{2}} e^{-\lambda[(u-U)^2 + \xi^2]}, \quad (4)$$

where  $\lambda = m/2k_B T$  and  $K$  is the internal degree of freedom. If we consider the first order approximation of Eq. (3) with respect to the collision time  $\tau$ , the distribution function  $f$  has the corresponding expansion,

$$f = g - \tau(g_t + u g_x) - \tau \phi g_u. \quad (5)$$

The first two terms in Eq. (5) describe the free transport of particles during the traveling time between two successive collisions. This expression is consistent with the Chapman-Enskog expansion for the Navier-Stokes solutions, and a dynamic viscous coefficient  $\mu = \tau p$  can be obtained [20, 21]. At the same time, the force acceleration distorts the distribution function in the velocity space with the following contributions to the macroscopic flow variables. Macroscopic variables are related with particle distribution function through velocity moments,

$$\mathbf{W} = \begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \psi f d\Xi,$$

$$p = \frac{1}{3} \int ((u-U)^2 + \xi^2) f d\Xi,$$

$$q = \frac{1}{2} \int (u-U) ((u-U)^2 + \xi^2) f d\Xi,$$

where  $d\Xi = dud\xi$  and  $\psi = (1, u, \frac{1}{2}(u^2 + \xi^2))^T$  is the vector of moments for collision invariants. For the moments of Maxwellian distribution  $\int u^\alpha \xi^\beta g d\Xi = \rho \langle u^\alpha \xi^\beta \rangle$ , it has the property that

$$\langle u^\alpha \xi^\beta \rangle = \langle u^\alpha \rangle \langle \xi^\beta \rangle.$$

For simplicity, let us consider a gas system with zero macroscopic velocity. In this case, the moments of Maxwellian distribution function are

$$\begin{aligned} \langle u^0 \rangle &= 1, \\ \langle u^1 \rangle &= 0, \\ \langle u^2 \rangle &= \frac{1}{2\lambda}, \\ \langle u^3 \rangle &= 0, \\ \langle u^4 \rangle &= \frac{3}{4\lambda^2}, \\ \langle \xi^2 \rangle &= \frac{K}{2\lambda}. \end{aligned} \quad (6)$$

The net contribution of macroscopic variables from the external forcing term can be written as

$$\Delta \mathbf{W} = \begin{pmatrix} \Delta \rho \\ \Delta \rho U \\ \Delta \rho E \end{pmatrix} = \int \psi (-\tau \phi g_u) d\Xi,$$

$$\Delta p = \frac{1}{3} \int (u^2 + \xi^2) (-\tau \phi g_u) d\Xi,$$

$$\Delta q = \frac{1}{2} \int u (u^2 + \xi^2) (-\tau \phi g_u) d\Xi.$$

If the forcing term  $\phi$  and the collision time  $\tau$  are viewed as local constants, and the exact Maxwellian distribution in Eq. (4) is used to evaluate its velocity derivative, we have the following relations,

$$\Delta \mathbf{W} = \begin{pmatrix} \Delta \rho \\ \Delta \rho U \\ \Delta \rho E \end{pmatrix} = 2\tau\phi\lambda \int \psi u g d\Xi = 2\tau\phi\lambda\rho \begin{pmatrix} \langle u^1 \rangle \\ \langle u^2 \rangle \\ \frac{1}{2} (\langle u^3 \rangle + \langle u\xi^2 \rangle) \end{pmatrix},$$

$$\Delta p = \frac{2}{3} \tau \phi \lambda \int u (u^2 + \xi^2) g d\Xi = \frac{2}{3} \tau \phi \lambda \rho (\langle u^3 \rangle + \langle u\xi^2 \rangle),$$

$$\Delta q = \tau \phi \lambda \int u^2 (u^2 + \xi^2) g d\Xi = \tau \phi \lambda \rho (\langle u^4 \rangle + \langle u^2 \xi^2 \rangle).$$

For a monatomic gas with internal degree of freedom  $K = 2$  for the random particle motion in the  $y$  and  $z$  directions, based on the moments in Eq. (6), we get

$$\Delta \mathbf{W} = \begin{pmatrix} \Delta \rho \\ \Delta \rho U \\ \Delta \rho E \end{pmatrix} = \begin{pmatrix} 0 \\ \tau \phi \rho \\ 0 \end{pmatrix}, \quad (7)$$

$$\Delta p = 0, \quad (8)$$

$$\Delta q = 1.25 \frac{\tau \phi \rho}{\lambda}. \quad (9)$$

The Eq. (7), (8) and (9) present a quantitative contribution of external force field on the macroscopic flow variables, which isn't included in the traditional Navier-Stokes equations. It is clear that there exists contribution to the macroscopic flow velocity and the heat flux from the external forcing term. Between two successive collisions, the particles get acceleration and enhanced velocity, resulting in a macroscopic mass and energy transport along the direction of external force. In the continuum flow regime with intensive particle collisions, the collision time  $\tau$  tends to zero, and the influence of external force field can be omitted. However, at a limited particle collision time  $\tau$  and non-vanishing local Knudsen number, the external forcing term does effect the transport, especially in the transition regime. It is noted that the above analysis is based on the near-equilibrium assumption. With the increment of degree of rarefaction, even strong non-equilibrium effect is expected to appear.

### III. WELL-BALANCED UNIFIED GAS-KINETIC SCHEME

The well-balanced unified gas-kinetic scheme is a direct modeling on the length scale of cell size and time scale of local time step for the construction of corresponding governing equations in such scales. With the notation of cell averaged distribution function

$$f_{x_i, y_j, t^n, u_k, v_l} = f_{i,j,k,l}^n = \frac{1}{\Omega_{i,j}(\vec{x})\Omega_{k,l}(\vec{v})} \int_{\Omega_{i,j}} \int_{\Omega_{k,l}} f(x, y, t^n, u, v) d\vec{x} d\vec{v},$$

the update of macroscopic conservative variables and the particle distribution function are coupled in the following way,

$$\mathbf{W}_{i,j}^{n+1} = \mathbf{W}_{i,j}^n + \frac{1}{\Omega_{i,j}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_r dt + \frac{1}{\Omega_{i,j}} \int_{t^n}^{t^{n+1}} \mathbf{G}_{i,j} dt, \quad (10)$$

$$\begin{aligned} f_{i,j,k,l}^{n+1} = & f_{i,j,k,l}^n + \frac{1}{\Omega_{i,j}} \int_{t^n}^{t^{n+1}} \sum_{r=1} u_r \hat{f}_r(t) \Delta S_r dt \\ & + \frac{1}{\Omega_{i,j}} \int_{t^n}^{t^{n+1}} \int_{\Omega_{i,j}} Q(f) d\vec{x} dt + \frac{1}{\Omega_{i,j}} \int_{t^n}^{t^{n+1}} \int_{\Omega_{i,j}} G(f) d\vec{x} dt, \end{aligned} \quad (11)$$

$$\mathbf{G}_{i,j} = \int_{\Omega_{k,l}} \left( -\phi_x \Delta t \frac{\partial}{\partial u} f_{i,j,k,l} - \phi_y \Delta t \frac{\partial}{\partial v} f_{i,j,k,l} \right) \psi du dv d\xi, \quad (12)$$

$$\begin{aligned} Q(f) &= \frac{f_{i,j,k,l}^+ - f_{i,j,k,l}^{n+1/2}}{\tau}, \\ G(f) &= -\phi_x \frac{\partial}{\partial u} f_{i,j,k,l}^{n+1} - \phi_y \frac{\partial}{\partial v} f_{i,j,k,l}^{n+1}. \end{aligned} \quad (13)$$

where  $\psi = (1, u, v, \frac{1}{2}(u^2 + v^2 + \xi^2))^T$  is the vector of moments for collision invariants, and  $\vec{\phi} = \phi_x \vec{i} + \phi_y \vec{j}$  is the external force acceleration. The implementation of the full Boltzmann collision term can be done as well when the time step is on the order of particle collision time [8]. However, if the time step is a few times of the local particle collision time, the use of kinetic model equation is accurately enough because the accumulating physical effect in a multiple particle collision time scale is not sensitive to the individual particle collision anymore.

The conservative variables are updated first, with  $\mathbf{F}_r$  being the fluxes of conservative flow variables and  $\mathbf{G}_{i,j}$  the source term from external force. The updated macroscopic variables can be used for the construction of the equilibrium state in  $Q(f)$  at  $t^{n+1}$  time step, and the derivatives of particle velocity in  $G(f)$  are evaluated via implicit upwind finite difference method in the discretized velocity space.

The BGK-type kinetic model is used to evaluate the interface distribution function  $f_r$ . The model equation with external force term in the two-dimensional Cartesian coordinate system is

$$f_t + u f_x + v f_y + \phi_x f_u + \phi_y f_v = \frac{g - f}{\tau}, \quad (14)$$

where  $\tau = \mu/p$  is the particle collision time.

In the unified scheme, at the center of a cell interface  $(x_{i+1/2}, y_j)$  the solution  $f_{i+1/2,j,k,l}$  is constructed from the integral solution of Eq. (14). With the notations  $x_{i+1/2} = 0, y_j = 0$  at  $t^n = 0$ , the time-dependent interface distribution function writes

$$\begin{aligned} f(0, 0, t, u_k, v_l, \xi) &= \frac{1}{\tau} \int_0^t g(x', y', t', u'_k, v'_l, \xi) e^{-(t-t')/\tau} dt' \\ &\quad + e^{-t/\tau} f_0(x^0, y^0, 0, u_k^0, v_l^0, \xi), \end{aligned} \quad (15)$$

where  $x' = -u'_k(t-t') - \frac{1}{2}\phi_x(t-t')^2$ ,  $y' = -v'_l(t-t') - \frac{1}{2}\phi_y(t-t')^2$ ,  $u'_k = u_k - \phi_x(t-t')$ , and  $v'_l = v_l - \phi_y(t-t')$  are the trajectories in physical and velocity space, and  $(x^0, y^0, u_k^0, v_l^0) = (-(u_k - \phi_x t) - \frac{1}{2}\phi_x t^2, -(v_l - \phi_y t) - \frac{1}{2}\phi_y t^2, u_k -$

$\phi_x t, v_l - \phi_y t$ ) is the initial location in physical and velocity space for the particle which passes through the cell interface at time  $t$ . The time accumulating effect from the external forcing term on the time evolution of the particle distribution function is explicitly taken into consideration.

To the second order accuracy, the initial gas distribution function  $f_0$  is reconstructed as

$$f_0(x, y, 0, u_k, v_l, \xi) = \begin{cases} f_{i+1/2,j,k,l}^L + \sigma_{i,j,k,l}x + \theta_{i,j,k,l}y, & x \leq 0, \\ f_{i+1/2,j,k,l}^R + \sigma_{i+1,j,k,l}x + \theta_{i+1,j,k,l}y, & x > 0, \end{cases}$$

where  $f_{i+1/2,j,k,l}^L$  and  $f_{i+1/2,j,k,l}^R$  are the reconstructed initial distribution functions at the left and right hand sides of a cell interface. The van Leer limiter is used in the reconstruction.

The equilibrium distribution function around a cell interface is constructed as

$$g = g_0 [1 + (1 - H[x])a^L x + H[x]a^R x + by + At],$$

where  $g_0$  is the Maxwellian distribution at  $(x = 0, t = 0)$ . Here the coefficients  $a^L, a^R$ , and  $A$  are from the Taylor expansion of a Maxwellian,

$$\begin{aligned} a^{L,R} &= a_1^{L,R} + a_2^{L,R}u + a_3^{L,R}v + a_4^{L,R}\frac{1}{2}(u^2 + v^2 + \xi^2) = a_\alpha^{L,R}\psi_\alpha, \\ b &= b_1 + b_2u + b_3v + b_4\frac{1}{2}(u^2 + v^2 + \xi^2) = b_\alpha\psi_\alpha, \\ A &= A_1 + A_2u + A_3v + A_4\frac{1}{2}(u^2 + v^2 + \xi^2) = A_\alpha\psi_\alpha. \end{aligned}$$

The coefficients above can be evaluated from the spatial distribution of conservative variables on both sides of the cell interface and the compatibility condition. After all the coefficients are determined, the time dependent interface distribution function becomes

$$\begin{aligned} f(0, 0, t, u_k, v_l, \xi) &= (1 - e^{-t/\tau})g_0 \\ &+ \left(\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right)a^{L,R}u_kg_0 \\ &- \left[\tau\left(\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right) + \frac{1}{2}t^2e^{-t/\tau}\right]a^{L,R}\phi_xg_0 \\ &+ \left(\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right)bv_lg_0 - \left[\tau\left(\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right) + \frac{1}{2}t^2e^{-t/\tau}\right]b\phi_yg_0 \\ &+ \tau\left(t/\tau - 1 + e^{-t/\tau}\right)Ag_0 \\ &+ e^{-t/\tau}\left[\left(f_{i+1/2,k^0,l^0}^L + \left(-(u_k - \phi_x t)t - \frac{1}{2}\phi_x t^2\right)\sigma_{i,k^0,l^0}\right.\right. \\ &\quad \left.+\left(-(v_l - \phi_y t)t - \frac{1}{2}\phi_y t^2\right)\theta_{i,k^0,l^0}\right)H\left[u_k - \frac{1}{2}\phi_x t\right] \\ &\quad \left.+\left(f_{i+1/2,k^0,l^0}^R + \left(-(u_k - \phi_x t)t - \frac{1}{2}\phi_x t^2\right)\sigma_{i+1,k^0,l^0}\right.\right. \\ &\quad \left.+\left(-(v_l - \phi_y t)t - \frac{1}{2}\phi_y t^2\right)\theta_{i+1,k^0,l^0}\right)(1 - H\left[u_k - \frac{1}{2}\phi_x t\right]) \\ &= \tilde{g}_{i+1/2,j,k,l} + \tilde{f}_{i+1/2,j,k,l}, \end{aligned} \tag{16}$$

where  $\tilde{g}_{i+1/2,j,k,l}$  is related to equilibrium state integration and  $\tilde{f}_{i+1/2,j,k,l}$  is related to the initial non-equilibrium distribution. The flux of conservative variables can be constructed as

$$\mathbf{F}_{i+1/2,j} = \int_{\Omega_{k,l}} u_k f(0, 0, t, u_k, v_l, \xi) \psi d\Xi.$$

#### IV. NUMERICAL EXPERIMENTS ON THE NON-EQUILIBRIUM FLOW EVOLUTION

In this section, we are going to present and discuss several numerical experiments to illustrate the non-equilibrium flow behavior under external force field. The hard sphere (HS) monatomic perfect gas is employed in all test cases. Di-

dimensionless quantities are introduced with  $\hat{x} = x/L_\infty$ ,  $\hat{\rho} = \rho/\rho_\infty$ ,  $\hat{T} = T/T_\infty$ ,  $\hat{u} = u/(2RT_\infty)^{1/2}$ ,  $\hat{t} = t(2RT_\infty)^{1/2}/L_\infty$ ,  $\hat{p} = p/(2\rho_\infty RT_\infty)$ ,  $\hat{\phi} = \phi L_\infty/(2RT_\infty)$ . For simplicity, we will drop the hat notation henceforth.

### A. Static heat conduction

Consider a vertical column of gas in which a temperature gradient is maintained through the top and bottom boundary temperature condition. Instead of studying the Rayleigh-Bénard convection [22, 23], we confine us to a static heat conduction problem to evaluate the correlation between heat flux and external force field. With the external force along the negative  $y$ -direction, the NSF equations indicate the following relations,

$$\frac{\partial}{\partial y} p = -\rho g, \quad (17)$$

$$\frac{\partial}{\partial y} \left( \kappa(y) \frac{\partial}{\partial y} T \right) = 0. \quad (18)$$

As is analyzed in Section 2, the external forcing term will influence the heat evolution process, resulting in a deviation of the temperature and heat flux profile away from the above theoretical solution in Eq. (18).

In the simulation, unit Prandtl number  $Pr = 1.0$  of a monatomic gas is assumed. The reference Knudsen number is set as  $Kn_{ref} = 0.001, 0.075, 1.0$ , which defines the dynamic viscosity in the reference state via variable hard sphere model (VHS),

$$\mu_{ref} = \frac{5(\alpha + 1)(\alpha + 2)\sqrt{\pi}}{4\alpha(5 - 2\omega)(7 - 2\omega)} Kn_{ref}. \quad (19)$$

We choose  $\alpha = 1.0$  and  $\omega = 0.5$  to recover a hard sphere monatomic gas. The viscosity for the hard-sphere model is,

$$\mu = \mu_{ref} \left( \frac{T}{T_{ref}} \right)^\theta, \quad (20)$$

where  $T_{ref}$  is the reference temperature and  $\theta$  is the index related to HS model. In this case we adopt the value  $\theta = 0.72$ . The local collision time is evaluated with the relation  $\tau = \mu/p$ . The temperature ratio of the bottom hot wall to the top cold one is set up with  $r = T_h/T_c = 1.2$ . An external acceleration  $\phi_y$  is imposed along the direction of temperature gradient to the system with different values. The heat flux distribution along  $y$  axis is presented in Fig. 1.

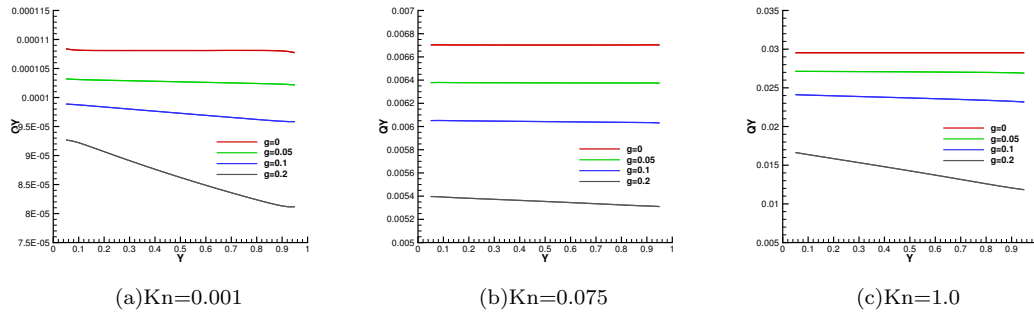


FIG. 1: Heat flux distribution in  $y$ -direction in different regimes.

It is observed that the heat flux is enhanced in the external force direction. In the near-equilibrium region with weak external force, the flux modification is proportional to the magnitude of the external force. The simulation results agree well with the predictive value in Eq. (9). In the convergent state, the heat flux is determined from

$$Q = Q_{fourier} + Q_{force}.$$

With the increment of reference Knudsen number and the magnitude of the external force, the contribution of heat flux from the forcing term is much more significant. Due to the non-equilibrium effect and large variation of the local

Knudsen number, the additional heat flux is no longer proportional to the magnitude of the external force. Now the spatial inhomogeneous heat flux is balanced by the macroscopic flow transport. As analyzed in Section 2, the gas under external force cannot be absolutely stationary. In the continuum limit, the velocity increment caused by the external force follows the relationship in Eq. (7), which is aligned with the force direction. However, in the transition regime, as shown in Fig. 2, the non-equilibrium flow transport can present a reversed velocity.

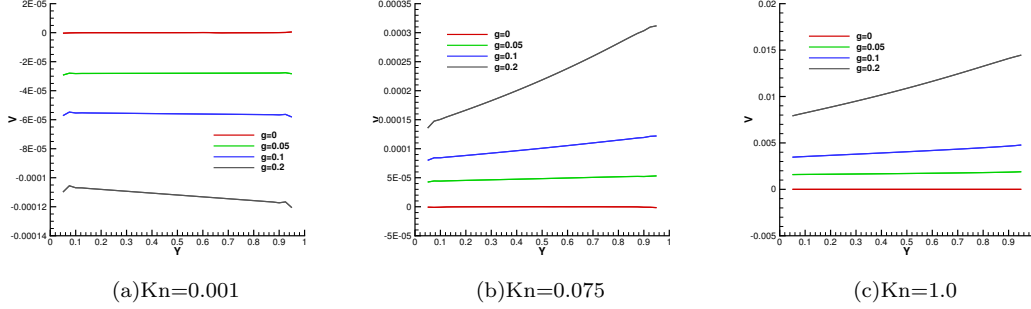


FIG. 2:  $V$ -velocity distribution in  $y$ -direction in different regimes.

The external forcing term may play an equivalent role as the temperature gradient in the determination of the heat flux. Fig. 3 shows the simulation result at a reference Knudsen number  $Kn_{ref} = 0.1$ , and external forcing acceleration  $\phi_y = -1.0$ . With the variation of local Knudsen number, the flow physics changes accordingly. In the region near the bottom wall, the temperature gradient contributes more to heat flux in comparison with the external forcing term, and the final heat flux in this region is still along the negative temperature gradient direction. However, at the upper rarefied region, the external forcing term dominates the heat transfer process, resulting the heat flux in the opposite direction. In the transition regime, the heat flux is associated with complicated non-equilibrium process.

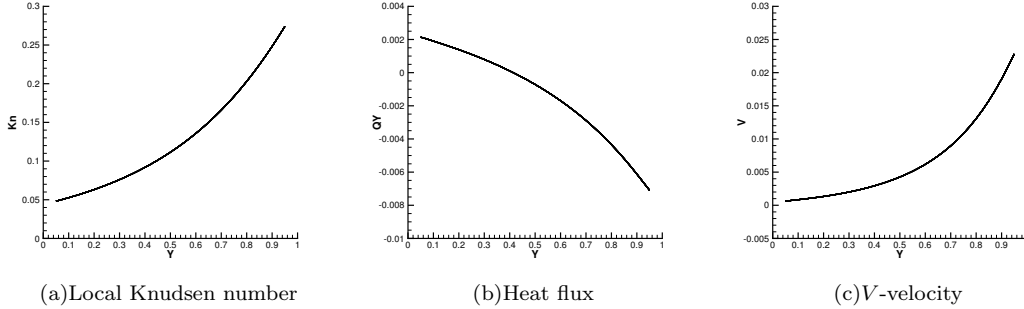


FIG. 3: Distribution of macroscopic quantities in  $y$ -direction with  $\phi_y = -1.0$  and  $Kn_{ref} = 0.1$ .

### B. Lid-driven cavity flow under external forcing field

Different from the previous case with the same direction for the temperature gradient and external force, the horizontal moving upper surface of the cavity will induce dissipative shear effect into the dynamic system under vertical external force field. The square cavity has four walls with length  $L = 1$ . The upper wall moves in tangential direction with a velocity  $U_w = 0.15$ . The external forcing acceleration is set up with  $\phi_y = 0.0, -0.1, -0.3, -0.5, -1.0$  respectively in the negative  $y$ -direction. The magnitude of gravity  $\phi_y$  is denoted by  $g$ . Non-dimensional Froude number can be defined in this system to quantify the relative importance of the upper wall's driving velocity and the effect of external force,

$$Fr = \frac{U_w}{\sqrt{gL}}. \quad (21)$$



The initial density and pressure are defined as

$$\rho(x, y, t = 0) = \exp(\phi_y y), p(x, y, t = 0) = \exp(\phi_y y),$$

and wall temperature is  $T_w = 2$ . Maxwell's diffusive reflecting boundary condition is used in the simulation. The Prandtl number of the gas is  $Pr = 0.67$ . The reference Knudsen number is selected as  $Kn_{ref} = 0.001, 0.075$ , which is defined by reference state at bottom of the cavity  $\rho_{ref} = 1.0$  and  $p_{ref} = 1.0$ . The computational domain is divided into  $45 \times 45$  uniform cells, and  $28 \times 28$  Gaussian points in velocity space.

### 1. Near equilibrium regime

In this case, the movement of upper surface and the external forcing term are two driving sources for the fluid motion. The initial hydrostatic distribution of density and pressure is perturbed by the upper wall's movement. Besides the viscous dissipation and heat conduction, the external force field participates in the flow and heat transport inside the cavity. Different from the non-equilibrium flow phenomena in the absence of external force, here the simple one large eddy topological structure covering the whole cavity domain may not necessarily appear due to the large density variation and different transport mechanism for different local Knudsen number flow. Fig. 4 presents the temperature contour along with the heat flux under different external forcing terms at  $Kn_{ref} = 0.001$ , and Fig. 5 shows the velocity distribution along the center lines. At a small magnitude of external force, there exists a single large eddy running through the whole cavity domain, and the distribution of  $U$ -velocity along the vertical center line is a monotonic curve. However, with the increment of the magnitude of external force, the flow pattern changes significantly. As presented in Fig. 6, with the relatively large external force, there is an obvious density variation along the vertical center line. In spite of the driving effect at the upper surface, the high density region around the bottom forms a "death flow region", and the eddy is restricted to the upper half domain of the cavity. Under this situation, an inflexion point appears in the  $U$ -velocity curve, leaving the lower part flow almost stationary. In fact, Fig. 6 shows that the flow in the upper region of the cavity stays in the transition regime, where profound non-equilibrium flow phenomena with a variation of local Knudsen number appear in such a gas dynamic system.

The heat transfer inside the cavity is closely coupled with flow transport. In the absence of external force, particle collisions at the top right corner result in a viscous heating at the macroscopic level, as shown in Fig. 4a. Due to intensive particle collisions, the expansion cooling at the top left corner is not obvious in this case, and the temperature around other three boundaries is almost uniform. This is consistent with the NS solutions in the continuum regime [8]. With an increment of external forcing term, the localized hot and cold spots move away from the corner regions, and propagate into the cavity. The penetration of the spots is related to the scale of the main eddy. From the results in Fig. 4 and 5, the center of the hot spot is located around the place where the negative  $U$ -velocity approaches to its maximum value, and the center of the cold spot locates a little bit higher than the hot one. At the current  $Kn_{ref} = 0.001$ , the particle distribution function will not deviate far from the Maxwellian equilibrium state. As analyzed in Section 2, the correlation between the heat flux and the external force is proportional to the magnitude of the forcing term. Although the heat flux is still aligned with the temperature gradient in the upper domain, the heat flux in the lower static region lines up with the direction of the force field. The adjustment of the particle distribution function due to the external forcing term provides the dominant mechanism for the non-equilibrium heat transport.

### 2. Transition regime

Now let us turn our attention to the case of fully transition regime at  $Kn_{ref} = 0.075$ . As shown in Fig. 7 and Fig. 8, the particle penetration and efficient mixing generates one large eddy in all cases. The stabilizing effect due to external force field is to reduce the rotating speed of the vortex. With the increment of external force, the velocity profile in Fig. 8 is flattened, indicating a weaker vortex motion.

Even with the similar main vortex structure, in the transition regime the external force field exerts a greater impact on the heat transfer process. As presented in Fig. 7, in the absence of external force field, the expansion cooling and viscous heating both have distinguishable contribution to the heat flux, which presents a phenomena for the heat flow from the cold to hot region. This observation is consistent with the DSMC simulation and unified scheme solution [8, 19]. With the increment of the external force, the heat transfer gradually turns into the vertical direction along with the forcing field. The hot spot moves downwards, while the cold region expands along the horizontal direction. As demonstrated, even with the viscous heating from the isothermal upper wall, the temperature decreases there due to the energy exchange among kinetic, internal, and potential one. The cooling of the upper zone may have the similar mechanism as the dynamic cooling in the atmosphere. In the case with  $\phi_y = -1.0$ , the heat flux is almost

parallel to the external force direction, and the heat transport from the upper cold region to the bottom hot region. This clearly indicates the gravity-thermal instability. In the transition regime, the external force plays an important role in the determination of non-equilibrium heat transport.

### C. Wave-type heat transfer

Based on the diffusion process in Fourier's law, the NSF equations can be used to describe the temperature evolution. Without considering the dissipation function from shear stress and the net work caused by the variation of pressure, in the absence of heat source or sink the energy conservation equation is,

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T). \quad (22)$$

The parabolic nature in the above equation implies an infinite propagation speed for the heat. A first attempt to solve this problem was carried out by Cattaneo [24], who suggested Fourier's heat flux  $\mathbf{q} = -\kappa \nabla T$  should be replaced by a more general rule,

$$\tau(T) \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\kappa \nabla T, \quad (23)$$

where  $\tau$  is the relaxation time which depends on the mechanism of heat transport. Although many other researchers also developed new equations, a universal heat conduction law is still far from complete. Macroscopic equations alone may not be possible to give a complete non-equilibrium description of transport process at all. The current UGKS is based on both macroscopic and microscopic scale flow evolution, where the degree of freedom for capturing non-equilibrium state and transport is not fixed and depends on the flow regime. In fact, if temperature is regarded as an internal energy, heat transfer could depend on a combination of many factors related to energy transformation, such as temperature gradient, stress tensor, compressibility, degree of rarefaction, and the contribution from external forcing term. In different flow regimes, these factors may play different role, which explains the existence of heat transport from cold to hot region in transition regime. In the kinetic scale, the particle transport and penetration take place for the thermal energy transport and dissipation. In the Navier-Stokes limit, the flow motion is approximately described by the movement of fluid elements, and energy exchange takes place only through the boundaries between the elements by diffusion process without particle penetration. Due to the instant interaction between fluid elements, the Fourier's law gives an arbitrary high propagating speed for the heat energy. Theoretically, all information propagated in a gas system must go through the particle collision and transport, the particle random velocity  $C_c \sim \sqrt{RT}$  determines the physical speed. Hence, the propagation speed of thermal disturbance cannot be far away from the above speed in the case with small fluid bulk velocity. In the transition regime, with the variation of local Knudsen number a much more complicated dynamic process will emerge in the determination of heat transfer.

Here we study the transient temperature evolution in two driven cavity cases to explore mechanism of heat transfer in different flow regimes. Fig. 9 presents the time evolved temperature contour inside the cavity at  $Kn_{ref} = 0.001$  and  $\phi_y = -0.1$ . Initially, both hot and cold spots generated at the upper surface permeate downwards through a "transport" process even the generated fluid velocity remains in the top region. When the localized hot and cool spots reach the bottom at  $t = 0.92$ , complex heat transport process appears. As presented in Fig. 10, with the stratified density distribution, the shearing generated flow motion stays in the top region, the tiny flow velocity at the bottom contributes marginally to the thermal energy transport there. Even at  $t = 3.99$ , the main eddy is still restricted in the upper half of the cavity, and the transverse flow velocity at the bottom is very weak. Although the heat diffusion smears the temperature gradient, the time variation of the temperature field around bottom indicates the wave-type thermal energy propagation. As shown in Fig. 9d to Fig. 9k, the thermal wave travels back and forth between opposite solid walls in the bottom region, where the localized hot and cold spots exchange locations a few times. Fig. 11 presents the time-series horizontal temperature distribution near the bottom wall, and the wave pattern of temperature evolution is fully demonstrated. With the wave reflection and transmission between two solid walls, the thermal wave is gradually dissipated. At end, two large temperature spots from the upper region move slowly downward with the main flow eddy.

For the case in the transition regime at  $Kn_{ref} = 0.075$  and  $\phi_y = -0.5$ , the results are presented in Fig. 12. Here the particle penetration speeds up the momentum and energy mixing, and the external force field plays a much more critical role. As shown in Fig. 13, the main eddy grows up quickly, and the particle transport dominates the heat and mass transfer. In this case, the high-temperature gas moves downwards smoothly with the swirling flow. After reaching the downside wall, the hot gas spreads moderately along with the convection, and forms a hot spot near the left corner in Fig. 12f. Although the dissipation process contributes much to the heat transfer now, the wave pattern of temperature variation is still observed. As shown in Fig. 14, after reflected by the solid wall, the thermal

wave transmits reversely from  $t = 1.59$  to  $t = 2.66$ . During this process, the localized hot spot is transporting against the flow velocity and moves to the right corner in Fig. 12g. It is noted that due to the increased collision time and particle penetration at this Knudsen number, the thermal wave speed is much reduced in comparison with the previous one. It takes about  $\Delta t = 1.07$  for the wave to travel across the bottom wall, while this process is finished in  $\Delta t = 0.40$  in the previous case. Actually, under external force field the propagation of thermal wave may be closely coupled with the gravitational wave, which needs further investigation. The amplitude of thermal wave here is one quarter of the one at  $Kn_{ref} = 0.001$ , indicating a much reduced wave energy. With increasing collision time and external force, the thermal wave is dissipated rapidly, and the localized hot and cold spots exchange locations only once. As a consequence, a stable temperature distribution is formed. So, it seems that the thermal wave propagating phenomenon is a complex dynamic process related to non-equilibrium mechanism in different flow regimes. Different wave patterns are expected to appear due to the relative importance of particle transport over diffusion. The current numerical experiments provide valuable observations for the theoretical modeling for the macroscopic thermal wave propagating equations.

## V. CONCLUSION

The gas dynamics under external force field is intrinsically a multiple scale flow problem due to large density variation and a changeable local Knudsen number. In this paper, based on the well-balanced unified gas-kinetic scheme we investigate the multiscale, non-equilibrium flow dynamics under external forcing in different flow regimes. For the near equilibrium flow, the contribution of the external force to the heat flux is analyzed based on the kinetic model equation, and verified numerically as well. At the same time, a detailed investigation for lid-driven cavity case has been conducted and the non-equilibrium flow evolution has been quantitatively evaluated. The dynamic effect of the external force on the flow pattern and heat transfer is presented. With the UGKS method, it is now possible to explore the physics in the non-equilibrium transition flow regime. The current study presents the following observations. The external force has great contribution to the heat flux and aligns the heat flow in the forcing direction. The enhanced heat transport from the forcing term may overtake the contribution from the temperature diffusion process, which determines the heat flow from the upper cold high gravitational potential region to the lower hot low potential region and triggers the gravity-thermal instability. In the transition regime, the thermal wave propagating phenomena under external forcing field have been observed and quantitatively evaluated. This provides a first hand data for the construction of generalized Fourier's law to take account of the limited thermal propagating speed. For a physical gas system under external force field, it is naturally a multiple scale flow problem with a large variation of local Knudsen number. The understanding of the multiscale non-equilibrium flow phenomena will have great help to our understanding to the earth's atmosphere environment.

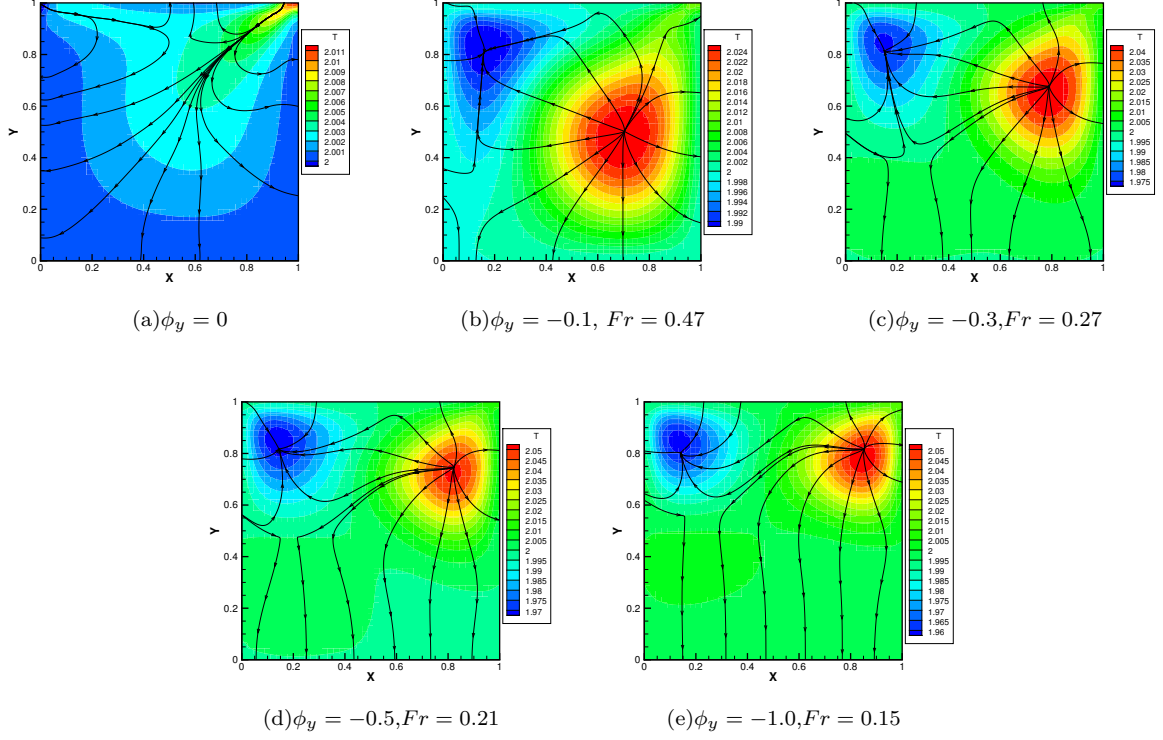
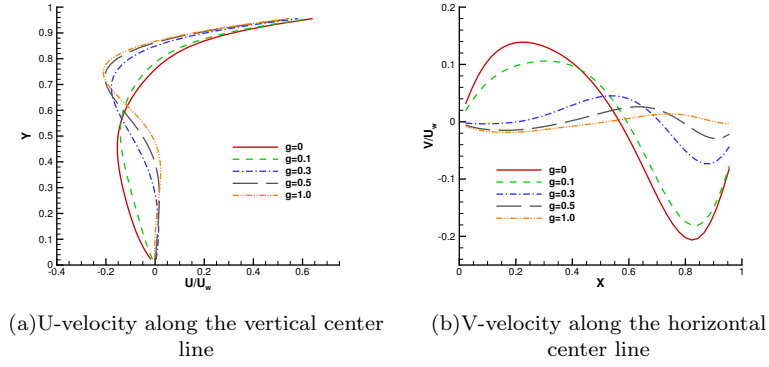
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FIG. 4: Temperature contour and heat flux with  $Kn_{ref} = 0.001$ .FIG. 5: Velocity distribution along the center line with  $Kn_{ref} = 0.001$ .

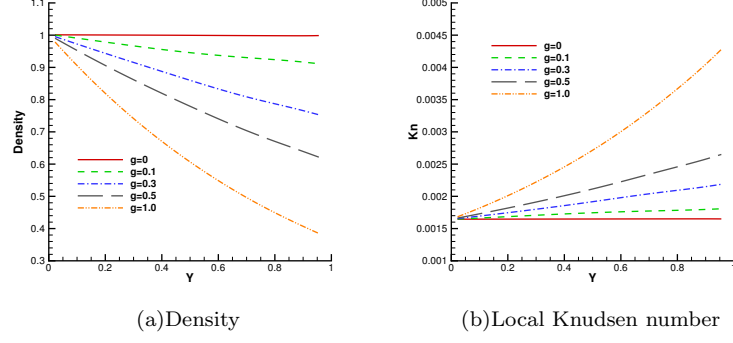


FIG. 6: Density and local Knudsen number distribution along the vertical center line with  $Kn_{ref} = 0.001$ .

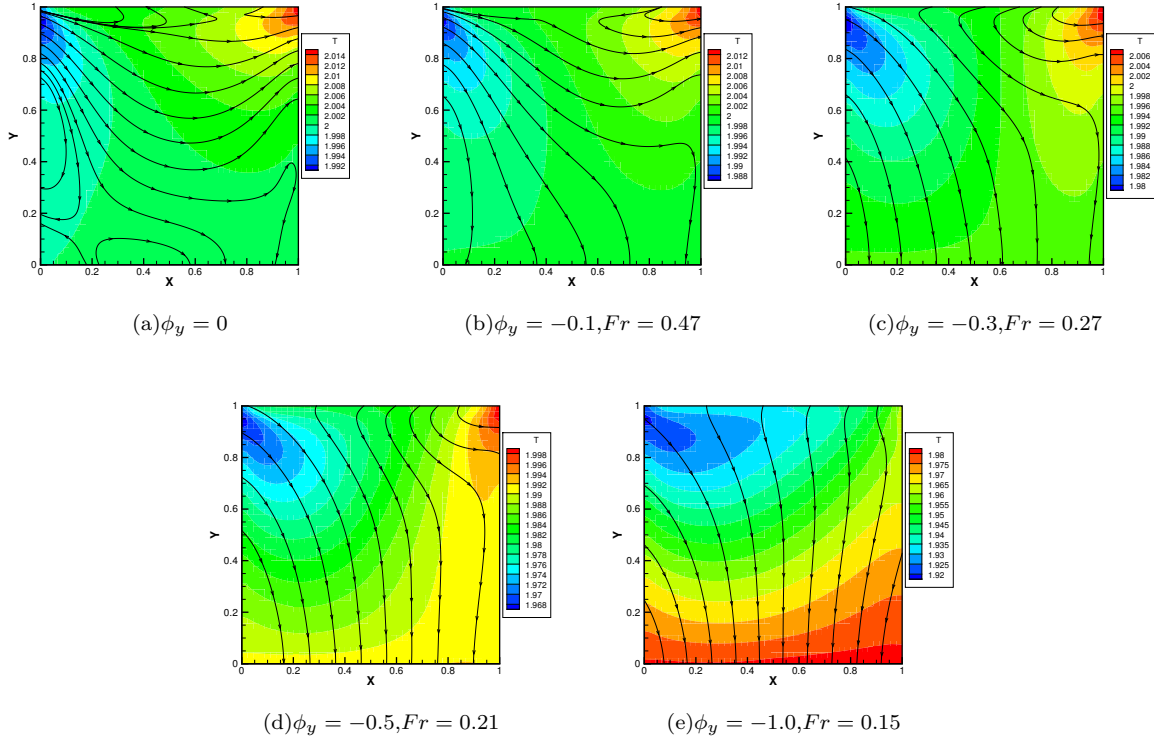


FIG. 7: Temperature contour and heat flux with  $Kn_{ref} = 0.075$ .

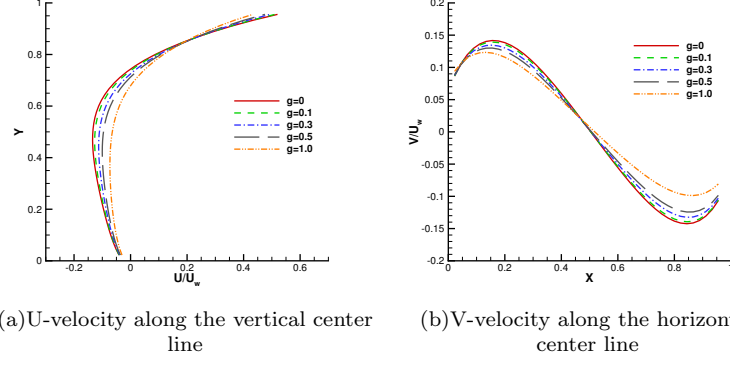


FIG. 8: Velocity distribution along the center line with  $Kn_{ref} = 0.075$ .

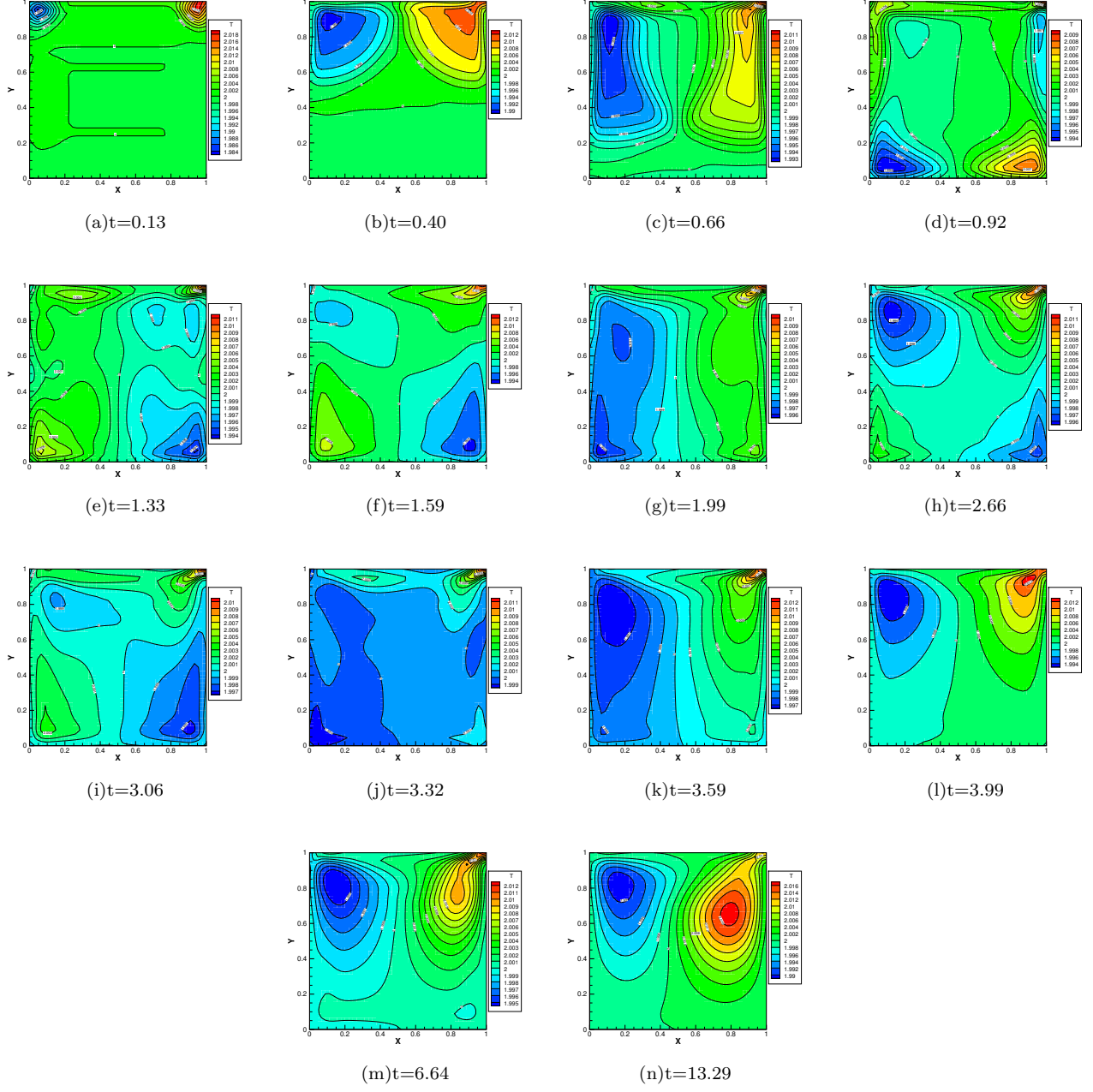


FIG. 9: Evolution of temperature with  $K n_{ref} = 0.001$  and  $\phi_y = -0.1$ .



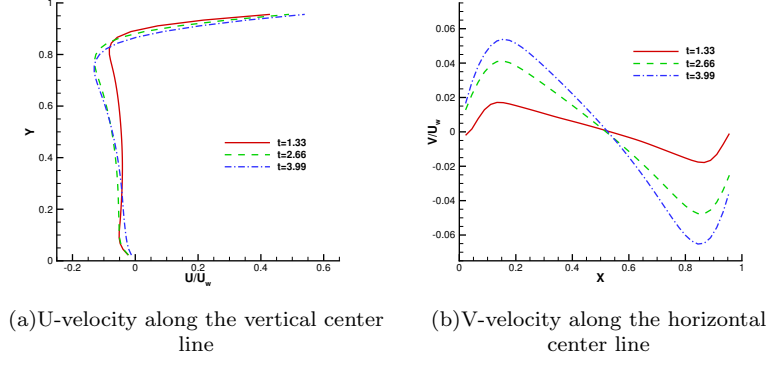


FIG. 10: Transient velocity distribution along the center line with  $Kn_{ref} = 0.001$  and  $\phi_y = -0.1$ .

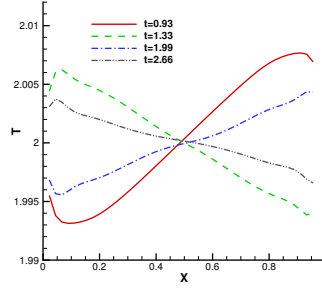


FIG. 11: Transient temperature distribution along horizontal direction near the bottom with  $Kn_{ref} = 0.001$  and  $\phi_y = -0.1$ .

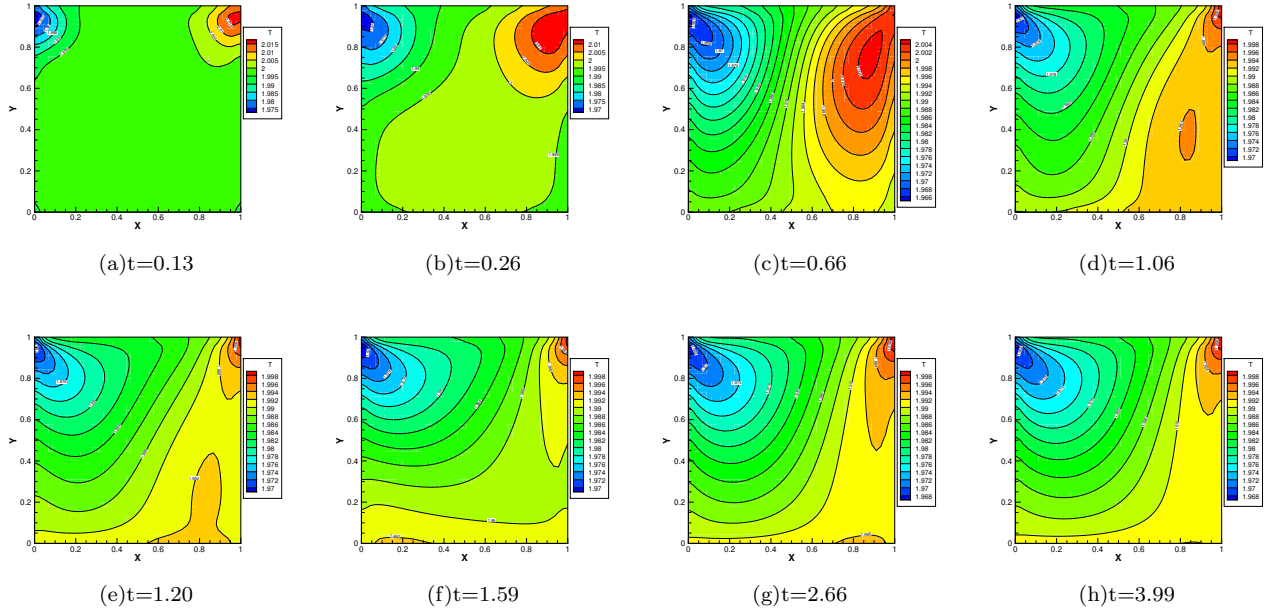


FIG. 12: Evolution of temperature with  $Kn_{ref} = 0.075$  and  $\phi_y = -0.5$ .

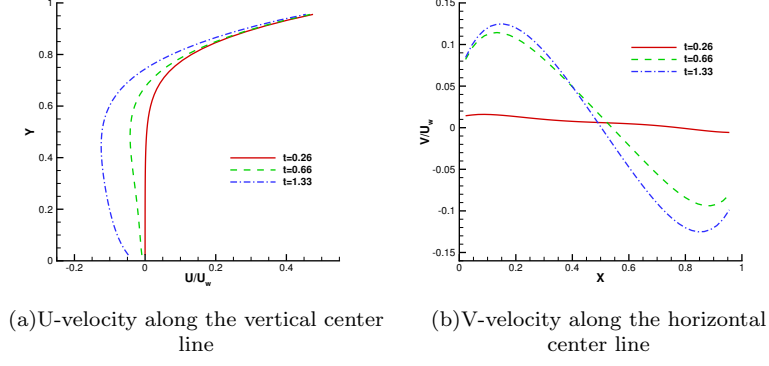


FIG. 13: Transient velocity distribution along the center line with  $Kn_{ref} = 0.075$  and  $\phi_y = -0.5$ .

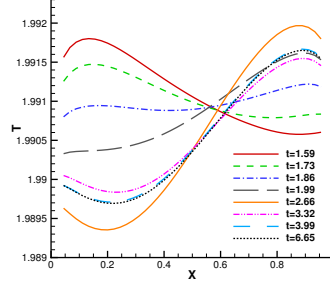


FIG. 14: Transient temperature distribution along horizontal direction near the bottom with  $Kn_{ref} = 0.075$  and  $\phi_y = -0.5$ .